

REPORT DOCUMENTATION PAGE

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DTS

MEMORANDUM FOR PRR (In-House Publication)

FROM: PROI (TI) (STINFO)

24 May 1999

SUBJECT: Authorization for Release of Technical Information, Control Number: AFRL-PR-ED-TP-FY99-0108
Gordon, Voth, Pachter, Boatz, "DoD High Performance Computing Challenge Project: New Materials Design"
Presentation (Public Release)



DoD High Performance Computing Challenge Project

New Materials Design

Prof. Mark S. Gordon, Iowa State University

Prof. Gregory Voth, University of Utah

Dr. Ruth Pachter, AFRL/MILPJ

Dr. Jerry Boatz, AFRL/PRS

DoD HPC Users Group Conference

Monterey, CA

7-11 June 1999

DISTRIBUTION STATEMENT A
Approved for Public Release
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New Materials Design

OUTLINE

1. Project Overview

- Atom-doped solid hydrogen and high energy density molecules as advanced rocket propellants
- “Explosive” annulenes as possible route to new nanostructural materials

2. Theoretical Methods, benchmarks

- Centroid Molecular Dynamics
- Ab initio electronic structure theory

3. Results

4. Future Directions



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10.31 kcal

OVERVIEW

1. Propellants

- Solid hydrogen doped with high energy species (e.g., atoms) offer revolutionary improvements in rocket propulsion over currently used LOX/LH₂ (SSME).
- High energy density molecules may improve performance of traditional solid and liquid propellants.

2. “Explosive” annulenes

- Precursors to carbon nanotubes, may provide route to heteroatomic nanostructural materials.



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COMPUTATIONAL METHODS

1. Centroid Molecular Dynamics (CMD*)

- Simulation method developed by Prof. Voth which properly treats quantum effects (e.g., zero point vibrational energy, tunneling). Essential for reliable characterization of solid hydrogen (low temperatures, light particles.)

2. Ab Initio Electronic Structure Theory (GAMESS*, G94, ACESII,...)

- Approximate solutions of Schrodinger equation applied to molecules. Prediction of molecular structures, energies, reaction pathways and stabilities, synthetic routes, spectroscopic constants, solvation effects, etc.

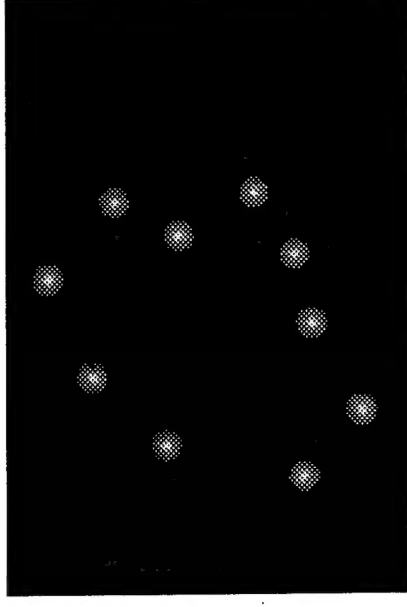
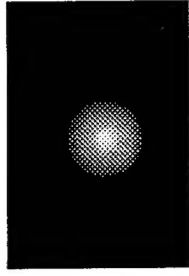
* CHSSI codes



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CENTROID MOLECULAR DYNAMICS

Simulation method based on path integral techniques for mapping quantum particles onto “polymer ring” of classical quasiparticles:



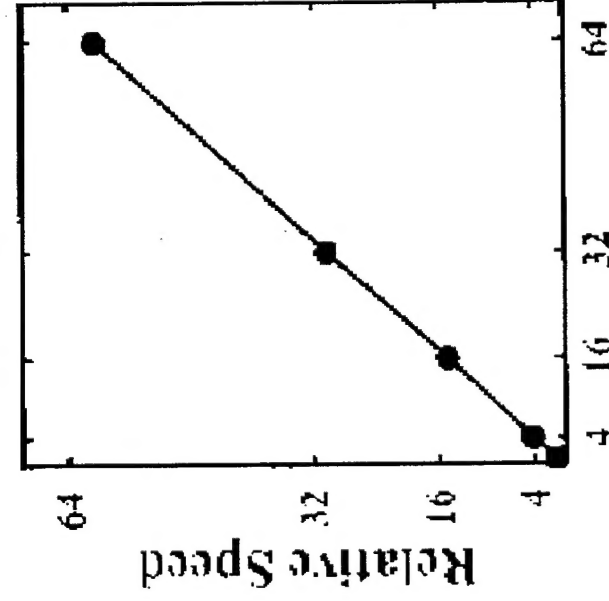
Each “real” particle is replaced by N ($50 < N < 500$) quasiparticles; classical dynamics done on collection of quasiparticles \Rightarrow natural, efficient parallelism.



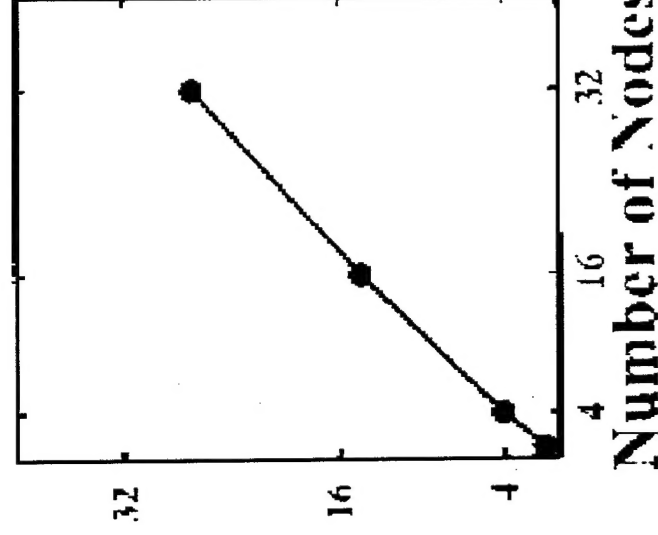
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Centroid Molecular Dynamics code shows linear scaling!

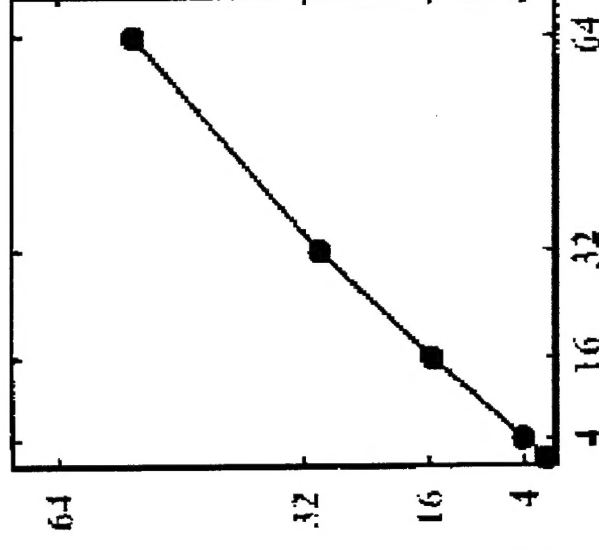
Cray T3E



SGI Origin 2000



IBM SP





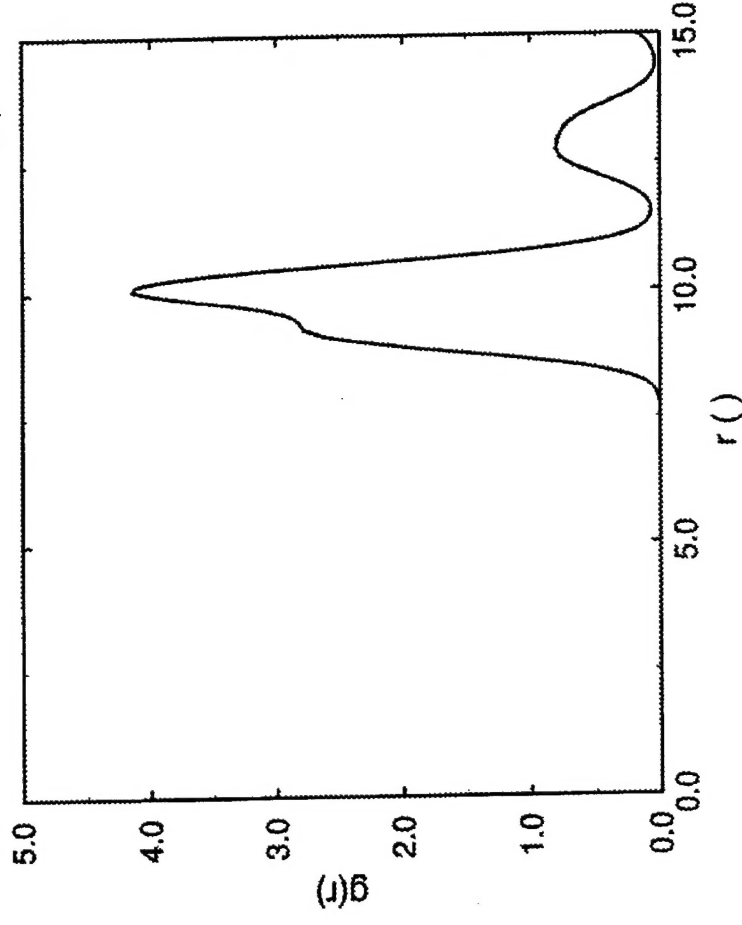
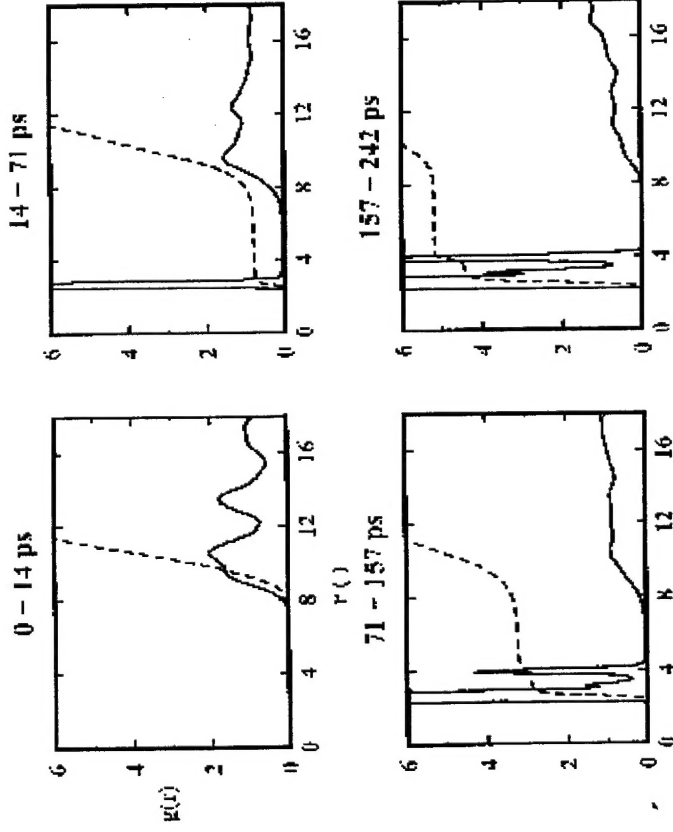
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3.3 % lithium atoms in
solid H_2 are stable for
only 10 picoseconds

6 % boron atoms in solid
 H_2 are stable for
nanoseconds

Computational requirements: 6 ps trajectory of 400-
atom system takes 10,000 node-hours on 120MHz SP

48 Lithium Atoms

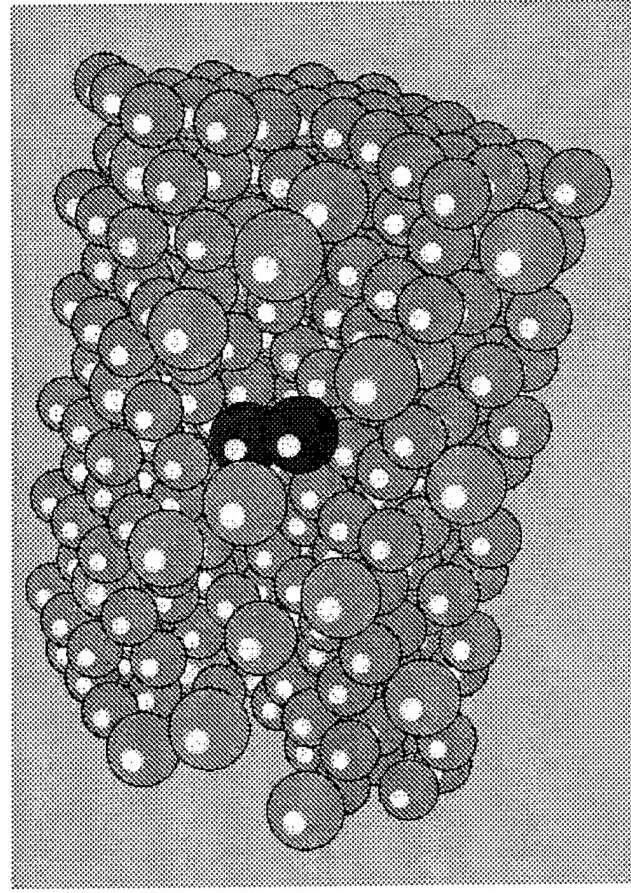




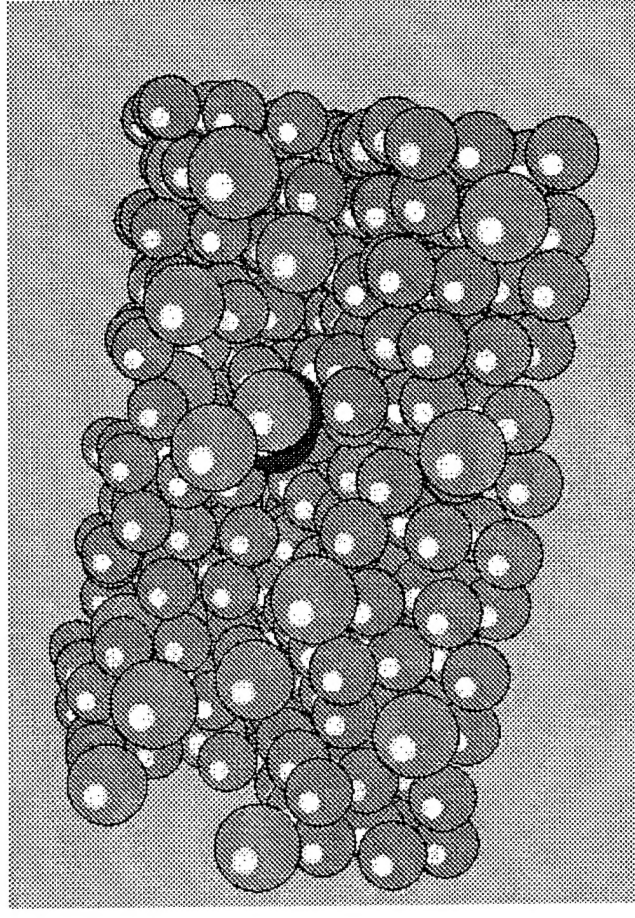
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6.25% boron atoms in solid *para*-hydrogen

Before reaction. Reacting boron atoms are shown in red. (Some hydrogens are hidden for viewing convenience.)



After reaction. (Note only local recombination of impurities!)



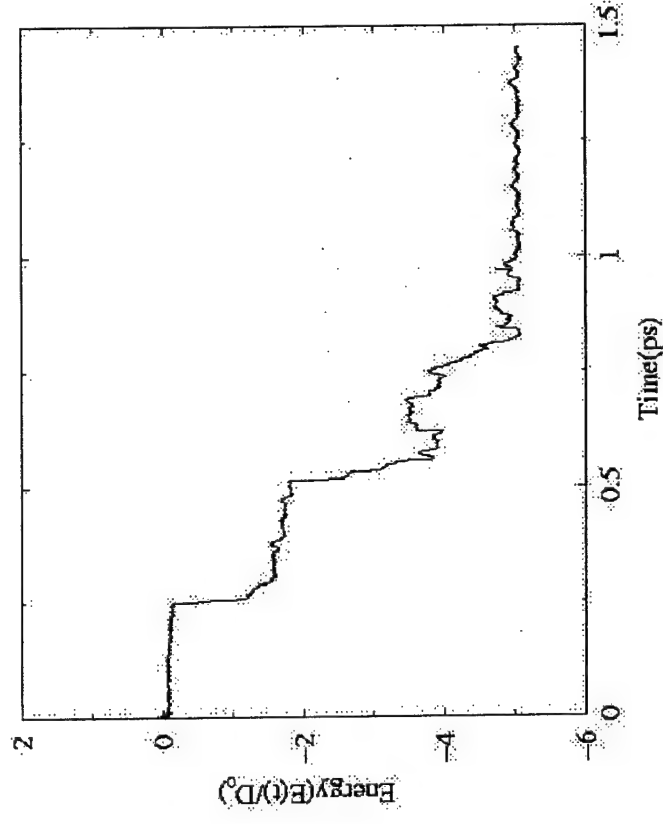
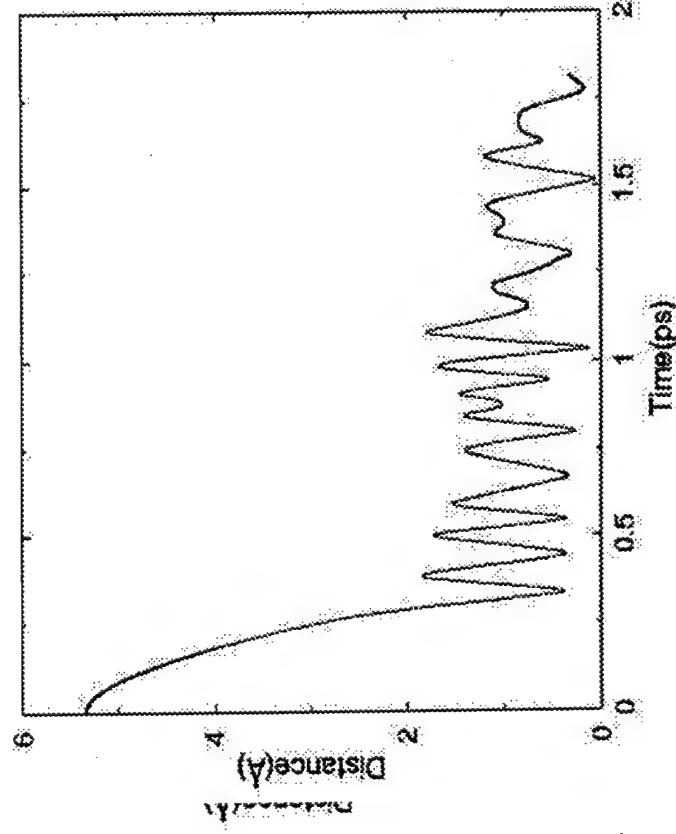


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6.25% boron atoms in solid *para*-hydrogen

Distance between two tagged boron atoms as a function of time.

Released energy as a function of time for the same system. D_0 is the boron-boron interaction well depth.





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Computational Approach in Electronic Structure Theory

Attempt to solve the time-independent Schrodinger equation for a molecule

$$\hat{H} \Psi(\mathbf{r}_e; \mathbf{R}_N) = E \Psi(\mathbf{r}_e; \mathbf{R}_N)$$

\hat{H} = quantum mechanical Hamiltonian operator

$$= -\sum_i \frac{1}{2} \nabla_i^2 - \sum_N \frac{1}{2M_N} \nabla_N^2 - \sum_i \sum_N \frac{Z_N}{R_{iN}} + \sum_i \sum_{j>i} \frac{1}{R_{ij}} + \sum_M \sum_{N>M} \frac{Z_M Z_N}{R_{MN}} +$$

E = total energy of the molecule

$\Psi(\mathbf{r}_e; \mathbf{R}_N)$ = molecular wavefunction



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Current Status of parallel GAMESS

	<u>RHF</u>	<u>ROHF</u>	<u>UHF</u>	<u>GVB</u>	<u>MCSCF</u>
Energy	cdp	cdp	cdp	cdp	cdp
Analytic Gradient	cdp	cdp	cdp	cdp	cdp
Numeric Hessian	cdp	cdp	cdp	cdp	cdp
Analytic Hessian	cdp	cdp	-	cdp	-
MP2 energy	cdp	cdP ₋	cdP ₋	-	c
MP2 gradient	cdP ₋	-	-	-	-
CI energy	cdp	cdp	-	cdp	cdp
CI gradient	cd	-	-	-	-

c = conventional disk storage of AO integrals

d= direct evaluation of AO integrals

p = parallel exection

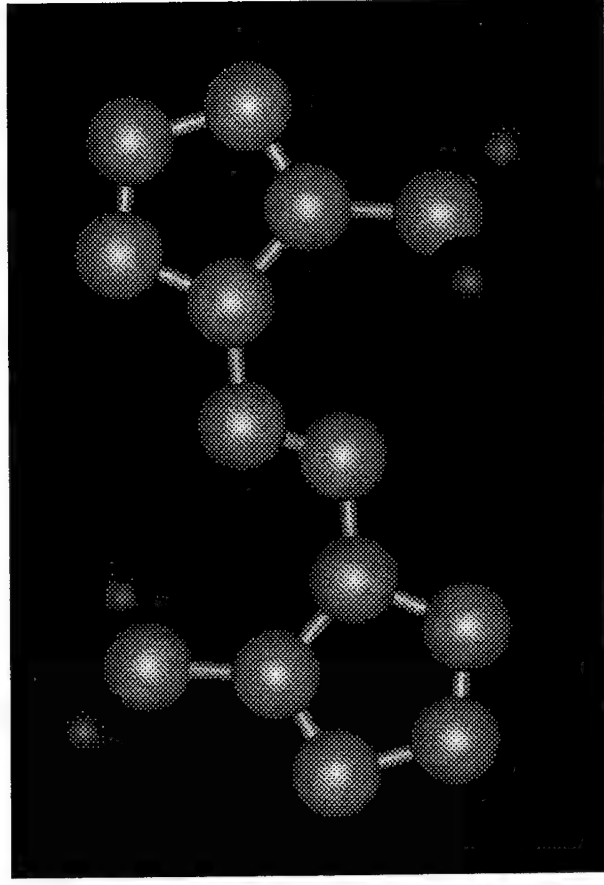
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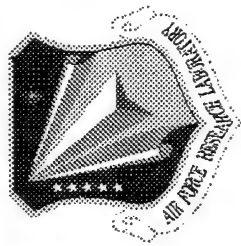


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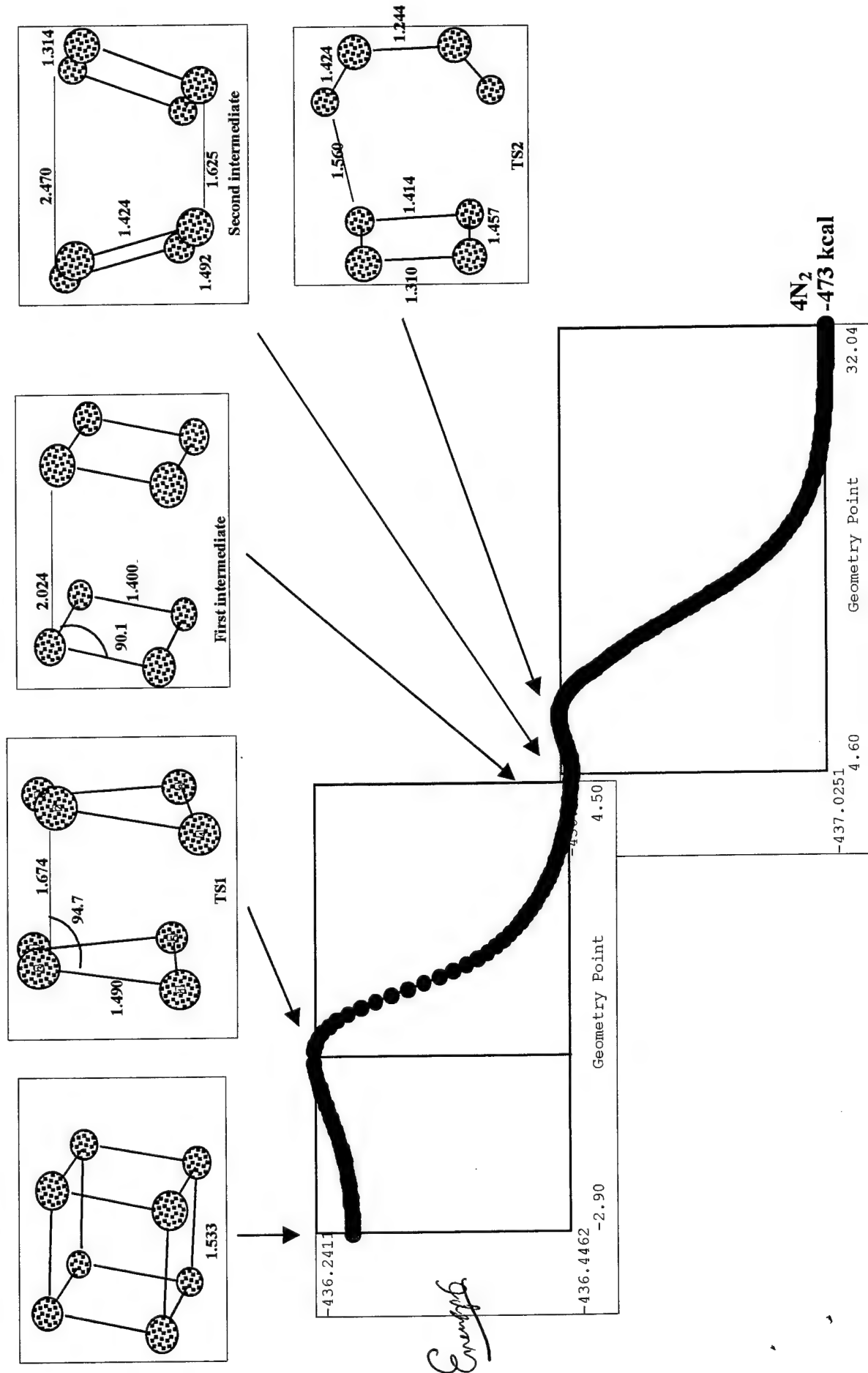
Calculated heat of formation (energy content relative to elements in their standard states) = 457 kcal/mol. Specific impulse (I_{sp}) = 329 sec.

I_{sp} of hydrazine = 240 seconds, I_{sp} of RP-1/LOX = 300 sec.



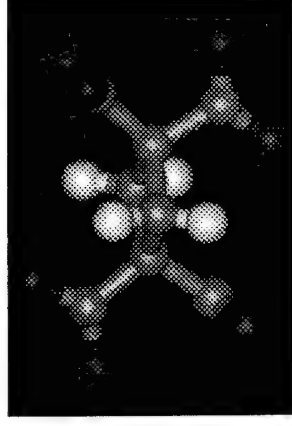


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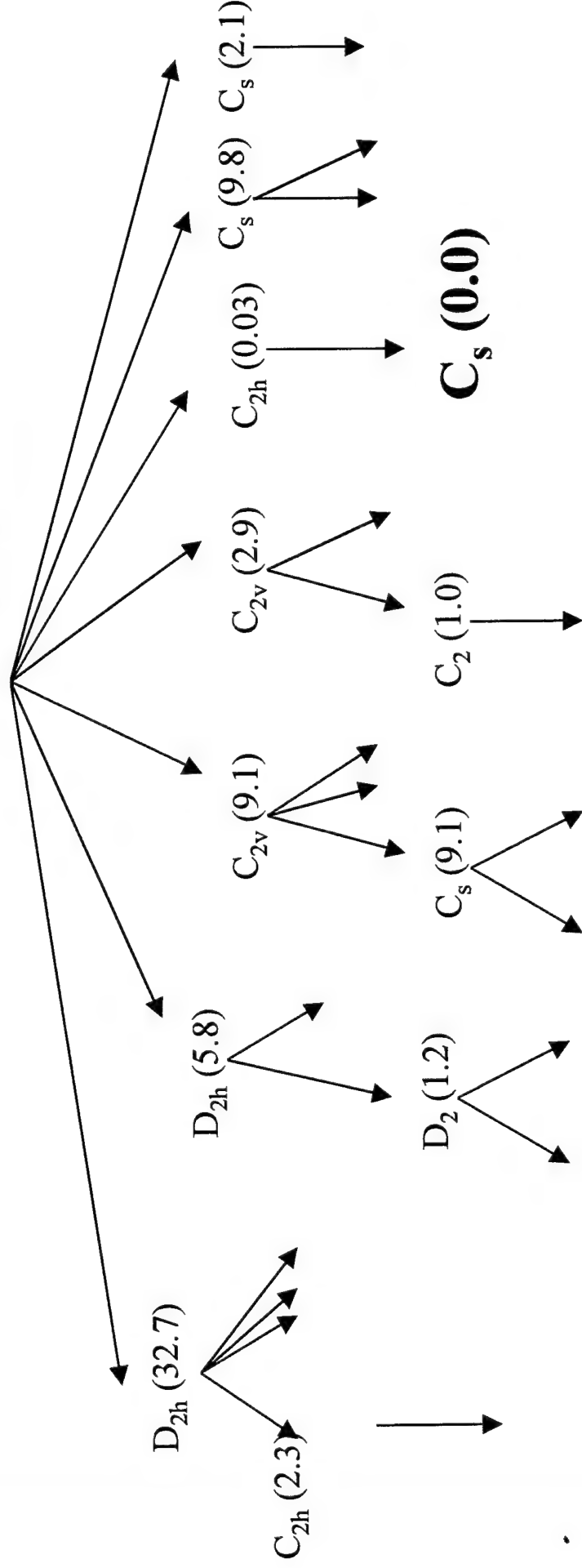




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Potential Energy Surfaces
can be very complicated

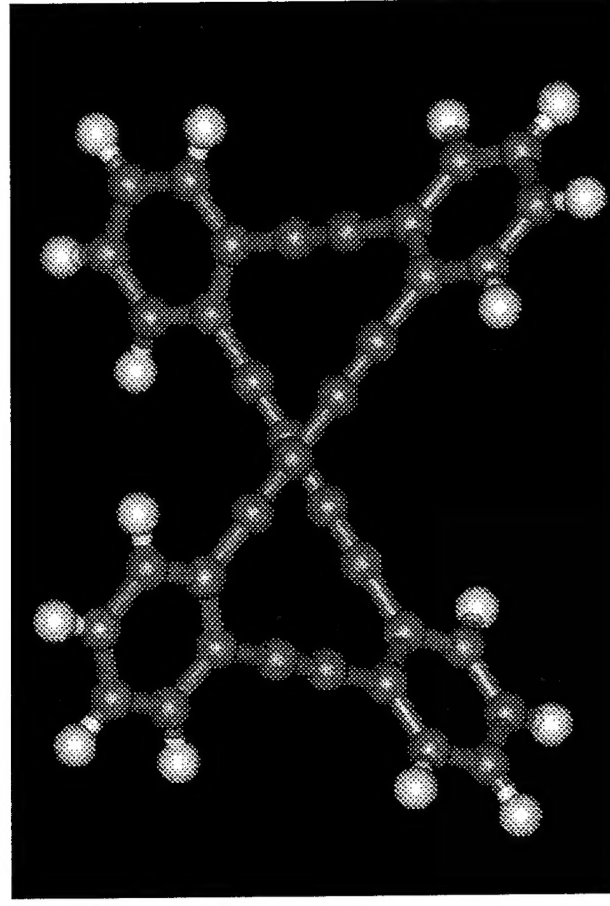
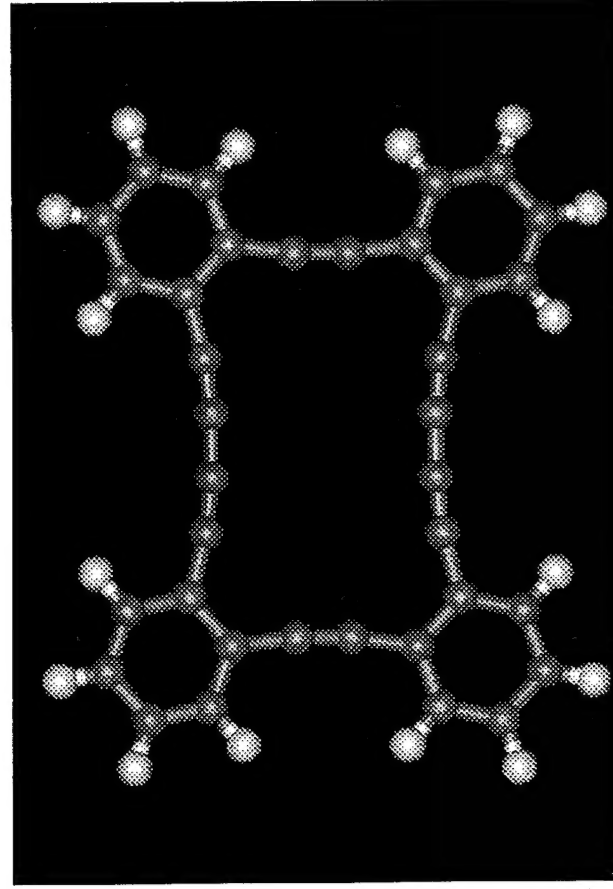




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“Explosive” Annulenes

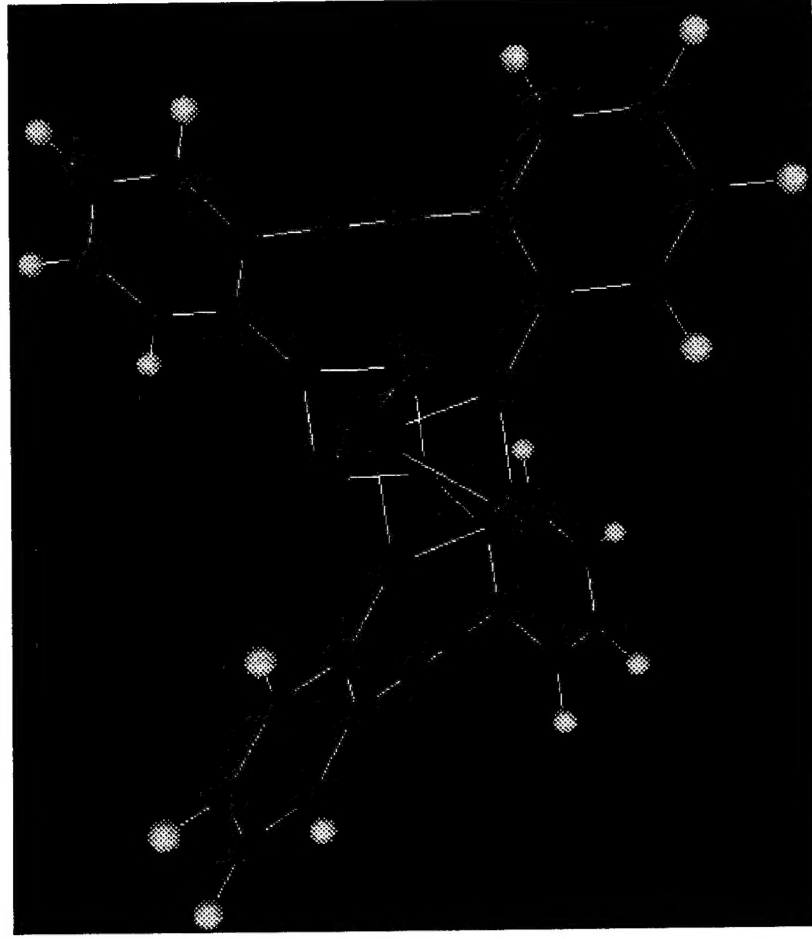
Decompose at 245°C , products include carbon nanotubes and “onion” fullerenes!





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**“Explosive” Annulenes: silicon derivatives:
possible route to heterofullerenes??**



Computational requirements:

Geometry optimization plus
numerical hessian: 10,000 node
hours/conformation

MP2 energies: 1.8 GW on
20 IBM SP nodes.



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CONCLUSIONS

2-10-85

1. In solid hydrogen, boron atoms are more stable than lithium atoms.
2. $C_2N_{12}O_4$ is superior to hydrazine and RP-1/LOX. Unresolved issues: kinetic stability, environmental interactions.
3. N_8 is probably too unstable for propulsion applications.
4. CHSSI has had a positive impact on CCM !!

2-10-85



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